

Exact mapping of periodic Anderson model to Kondo lattice model

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It is shown that the Kondo lattice model, for any finite coupling constant J , can be obtained exactly from the periodic Anderson model in an appropriate limit. The mapping allows a direct proof of the “large” Fermi volume for a nonmagnetic Fermi-liquid state of the Kondo lattice model.

The periodic Anderson model (PAM) and the Kondo lattice model (KLM) belong to the most intensively discussed many-body models in solid state physics. Both are believed to at least qualitatively describe important aspects of the extremely rich physics of so-called heavy-fermion systems^{1,2,3}. The properties of those systems are based on an interplay between rather localized f electrons and itinerant s , p or d conduction electrons. In the (non-degenerate) periodic Anderson model this is accounted for in a minimal way, considering non-degenerate f orbitals with intra-orbital Coulomb interactions and a non-degenerate conduction band with which the f orbitals are hybridized. The effective physics is often described in terms of the Kondo lattice model, where the f electrons are modelled as localized quantum-mechanical spins with an antiferromagnetic spin exchange with the conduction electrons via a coupling constant J . The KLM represents an effective model of the PAM in the so-called Kondo regime, which is relevant to heavy-fermion systems. In the Kondo regime the correspondence between the models is an approximate, perturbational one. It is known to become exact in the so-called Kondo limit of the PAM, which corresponds to the weak-coupling limit ($J \rightarrow 0$) of the KLM.

This relation between the KLM and the PAM was established a long time ago with the help of the Schrieffer-Wolff transformation^{4,5,6}, which was originally devised for the corresponding impurity models (single-impurity Anderson model⁷ and Kondo impurity model⁸) to show that those are related in a similar way. In a more recent paper Matsumoto and Ohkawa claimed for the single-impurity Anderson model and the Kondo impurity model an equivalence in a special “ s - d limit”, which differs from the Kondo limit⁹. Based on that, they inferred the same equivalence to hold between the PAM and the KLM in the case of infinite spatial dimensions. In this Letter we show that Matsumoto’s and Ohkawa’s s - d limit, in the following also called “extended Kondo limit”, can be used for a *direct* and *rigorous* mapping of the periodic Anderson model to the Kondo lattice model *in any dimensions*. Thus a fundamental relation between both models is established. In contrast with the (conventional) Kondo limit, the equivalence in the extended Kondo limit rigorously holds for any coupling J of the KLM.

The general fact of an exact mapping of the PAM to the KLM provides a general and rigorous answer to the long-standing issue of the “correct” Fermi-surface sum rule for the Kondo-lattice model. Luttinger’s theorem¹⁰, which states that the volume enclosed by the Fermi surface (“Fermi volume”) is (a) independent of the interaction strength as long as no phase transition occurs and (b) otherwise only related to the number of electrons, cannot be directly applied to the KLM since it is not a purely fermionic model. In particular it is a priori unclear, whether the localized spins can count as electrons in this context. With the exact mapping the *general* and *rigorous* answer can be given: the respective sum rule of the PAM is rigorously mapped to the KLM. We prove exemplarily that the Fermi volume of the KLM includes the number of localized spins (so-called “large” Fermi volume) if the system is in a nonmagnetic Fermi-liquid state. We thus confirm in a much simpler way the result of a recent topological proof by Oshikawa¹¹.

It is clear that via the extended Kondo limit it will be possible in future to obtain further analytical and computational results for the Kondo lattice model. Based on the rigorous mapping, any result of the PAM translates into one for the KLM, and any analytical or computational method for the PAM can be directly applied to the KLM.

This Letter is organized as follows: First, we review the correspondence between the Kondo regime of the periodic Anderson model and the weak-coupling regime of the Kondo lattice model. Then, the proof of rigorous equivalence between the KLM and the PAM in the extended Kondo limit is given. Finally, the direct proof of the large Fermi volume of the KLM which follows from the exact mapping is explained.

The Hamiltonian of the periodic Anderson model (PAM) is given by

$$H_{\text{PAM}} = \sum_{k\sigma} \epsilon_k n_{k\sigma} + \sum_{i\sigma} \epsilon_f n_{i\sigma}^f + U \sum_i n_{i\uparrow}^f n_{i\downarrow}^f + \sum_{ki\sigma} (V_k e^{-ikR_i} c_{k\sigma}^\dagger f_{i\sigma} + \text{H.C.}) . \quad (1)$$

$c_{k\sigma}^{(\dagger)}$ creates/annihilates a conduction electron (s electron) with momentum k , spin σ and one-particle energy ϵ_k . $f_{i\sigma}^{(\dagger)}$ is the creation/annihilation operator for an f electron at site R_i with energy ϵ_f . U is the Coulomb repulsion between f electrons at the same site (same f orbital). s -electron states are hybridized with f orbitals

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via hybridization matrix elements V_k .

The Hamiltonian of the Kondo lattice model (KLM) reads

$$H_{\text{KLM}} = \sum_{k\sigma} \epsilon_k n_{k\sigma} + \sum_{kk'i} J_{k'k} e^{-i(k'-k)R_i} \mathbf{S}_i \cdot \mathbf{s}_{k'k}. \quad (2)$$

The first part describes the conduction band. The second part stands for the interaction between localized quantum-mechanical spins \mathbf{S}_i of magnitude 1/2 and the spins of the conduction electrons $\mathbf{s}_{k'k} = \frac{1}{2} \sum_{\sigma'\sigma} c_{k'\sigma'}^\dagger \boldsymbol{\tau}_{\sigma'\sigma} c_{k\sigma}$ (with $\boldsymbol{\tau}$ representing the Pauli matrices). $J_{k'k}$ are the (antiferromagnetic) coupling constants ($J_{k'k} > 0$).

The Kondo regime of the PAM is a regime favourable for the formation of local f moments. A necessary condition clearly is that the energy of a singly (doubly) occupied f orbital lies below (above) the chemical potential: $\epsilon_f < 0$, $\epsilon_f + U > 0$. The energy distance to the chemical potential should be large compared with the hybridization so that fluctuations of f -orbital occupancy are small. This condition is usually formulated in terms of the width Γ of the virtual level of the single-impurity Anderson model^{3,5}:

$$\frac{\Gamma}{|\epsilon_f|}, \frac{\Gamma}{\epsilon_f + U} \ll 1, \quad (3)$$

where $\Gamma = \pi \rho_0 V^2$. ρ_0 is the density of states of the conduction band at the Fermi energy. V is the average hybridization ($V^2 = \{|V_k|^2\}_{\text{av}}$). Via the Schrieffer-Wolff transformation, the Kondo regime of the PAM is approximately mapped to the weak-coupling (small- J) regime of the Kondo lattice model. Assuming a constant density of states, the limit in which the mapping becomes exact (Kondo limit) is given by

$$\frac{V^2}{\epsilon_f}, \frac{V^2}{\epsilon_f + U} \longrightarrow 0. \quad (4)$$

The Kondo limit can be understood as $V \rightarrow 0$ or $|\epsilon_f|, \epsilon_f + U \rightarrow \infty$. Both corresponds to $J \rightarrow 0$ on the side of the Kondo lattice model¹⁶.

The extended Kondo limit (EKL), which leads to an exact mapping of the periodic Anderson model to the Kondo lattice model for arbitrary $J > 0$, is given by

$$\epsilon_f \equiv -\frac{U}{2} \\ U \rightarrow \infty, \quad V \rightarrow \infty \quad \text{with} \quad \frac{V^2}{U} \rightarrow \text{const.} \quad (5)$$

Note that $\epsilon_f \rightarrow -\infty$ as $U \rightarrow \infty$. The proof of exact mapping in the EKL consists of two steps. First, a finite Schrieffer-Wolff transformation is performed on the Hamiltonian of the PAM. Second, the consequences of the EKL on the transformed Hamiltonian are checked to rigorously prove that the only terms which remain relevant are those of the Kondo-lattice model.

The first three terms of H_{PAM} are denoted by H_0 , the hybridization term by H_V . To eliminate all terms first-order in V_k , a unitary transformation $\bar{H} = e^S H_{\text{PAM}} e^{-S}$ is performed with the condition $[S, H_0] = -H_V$. The required generator is

$$S = \sum_{k i \sigma} \left(\frac{V_k e^{-ikR_i}}{\epsilon_k - \epsilon_f - U} n_{i-\sigma}^f c_{k\sigma}^\dagger f_{i\sigma} + \frac{V_k e^{-ikR_i}}{\epsilon_k - \epsilon_f} (1 - n_{i-\sigma}^f) c_{k\sigma}^\dagger f_{i\sigma} \right) - \text{H.C.} \quad (6)$$

The transformed Hamiltonian is given by

$$\bar{H} = H_0 + H_2 + \frac{1}{3}[S, [S, H_V]] + \frac{1}{8}[S, [S, [S, H_V]]] + \dots, \quad (7)$$

with

$$H_2 \equiv \frac{1}{2}[S, H_V] = H_{\text{ex}} + H_{\text{dir}} + H_{\text{hop}} + H_{\text{ch}}, \quad (8)$$

where

$$H_{\text{ex}} = \frac{1}{2} \sum_{kk'i} J_{k'k} e^{-i(k'-k)R_i} (S_i^+ c_{k'\downarrow}^\dagger c_{k\uparrow} + S_i^- c_{k'\uparrow}^\dagger c_{k\downarrow} + S_i^z (c_{k'\uparrow}^\dagger c_{k\uparrow} - c_{k'\downarrow}^\dagger c_{k\downarrow})) \quad (9)$$

$$H_{\text{dir}} = \sum_{kk'i\sigma} (W_{k'k} - \frac{1}{4} J_{k'k} (n_{i\uparrow}^f + n_{i\downarrow}^f)) e^{-i(k'-k)R_i} c_{k'\sigma}^\dagger c_{k\sigma} \quad (10)$$

$$H_{\text{hop}} = - \sum_{kij\sigma} (W_{kk} - \frac{1}{4} J_{kk} (n_{i-\sigma}^f + n_{j-\sigma}^f)) e^{-ik(R_i - R_j)} * f_{j\sigma}^\dagger f_{i\sigma} \quad (11)$$

$$H_{\text{ch}} = -\frac{1}{2} \sum_{kk'i\sigma} V_{k'} V_k e^{-i(k'+k)R_i} ((\epsilon_{k'} - \epsilon_f - U)^{-1} - (\epsilon_{k'} - \epsilon_f)^{-1}) c_{k'-\sigma}^\dagger c_{k\sigma}^\dagger f_{i\sigma} f_{i-\sigma} + \text{H.C.} \quad (12)$$

with coupling constants

$$J_{k'k} = V_{k'} V_k^* \{ -(\epsilon_k - \epsilon_f - U)^{-1} - (\epsilon_{k'} - \epsilon_f - U)^{-1} + ((\epsilon_k - \epsilon_f)^{-1} + (\epsilon_{k'} - \epsilon_f)^{-1}) \}, \quad (13)$$

$$W_{k'k} = \frac{1}{2} V_{k'} V_k^* \{ (\epsilon_k - \epsilon_f)^{-1} + (\epsilon_{k'} - \epsilon_f)^{-1} \}. \quad (14)$$

The spin operators in (9) are given by $\mathbf{S}_i = \frac{1}{2} \sum_{\sigma'\sigma} f_{i\sigma'}^\dagger \boldsymbol{\tau}_{\sigma'\sigma} f_{i\sigma}$.

Assuming a conduction band of finite width, the norm of the generator in the EKL has the asymptotics

$$\|S\| \stackrel{\text{EKL}}{\propto} \frac{V}{U}. \quad (15)$$

With $\|H_V\| \propto V$ and $V \stackrel{\text{EKL}}{\propto} \sqrt{U}$ it follows that all higher commutators in (7), starting at the order V^3/U^2 , exactly vanish in the EKL,

$$[S, [S, H_V]], [S, [S, [S, H_V]]], \dots \stackrel{\text{EKL}}{\longrightarrow} 0, \quad (16)$$

and it is sufficient to consider the EKL of the remaining Hamiltonian $\bar{H}' \equiv H_0 + H_2$.

It is important to note that one cannot proceed with the original argument given by Schrieffer and Wolff for the Kondo regime of the single-impurity Anderson model⁴. The reason is that apart from H_{ch} also H_{hop} changes the number of f electrons at given sites. H_{hop} connects the subspace of single f occupancy with the subspaces of zero and double occupancy. Therefore, the Hilbert space cannot be separated at this stage. To prove an effective fixing of f occupation, one needs to apply a different and more formal line of argumentation.

We denote the s and f electron parts of H_0 separately,

$$H_0^s = \sum_{k\sigma} \epsilon_k n_{k\sigma}, \quad H_0^f = \sum_{i\sigma} \epsilon_f n_{i\sigma}^f + U \sum_i n_{i\uparrow}^f n_{i\downarrow}^f. \quad (17)$$

In the EKL the different parts of \bar{H}' behave as:

$$\|H_0^s\| \propto \mathcal{W} = \text{const.} \quad (18)$$

$$\|H_2\| \propto \tilde{J} \equiv \frac{V^2}{U} = \text{const.} \quad (19)$$

$$\|H_0^f\| \propto U \xrightarrow{\text{EKL}} \infty. \quad (20)$$

\mathcal{W} is the width of the conduction band. Obviously, with respect to \bar{H}' the EKL is equivalent to just taking the limit $U \rightarrow \infty$ (and $\epsilon_f \equiv -\frac{U}{2} \rightarrow -\infty$). V needs not to be considered explicitly since it only appears within the ratio $V^2/U \equiv \tilde{J}$, which is a constant in the EKL.

Let us consider \bar{H}' and its eigenstates as functions of the three parameters \mathcal{W} , \tilde{J} and U . It is clear that the eigenstates $\{|\Psi(\mathcal{W}, \tilde{J}, U)\rangle\}$ actually only depend on the ratios \mathcal{W}/U and \tilde{J}/U . Therefore, in the EKL ($U \rightarrow \infty$) each eigenstate $|\Psi\rangle$ of \bar{H}' approaches an eigenstate $|\Psi^0\rangle$ of H_0^U :

$$|\Psi(\mathcal{W}, \tilde{J}, U)\rangle \xrightarrow{U \rightarrow \infty} |\Psi(0, 0, U')\rangle \equiv |\Psi^0\rangle \quad (21)$$

with arbitrary U' . Note that the states $\{|\Psi^0\rangle\}$ that are approached in the EKL are highly non-trivial superpositions of trivial degenerate eigenstates of H_0^U . Still, they can be grouped into two classes: first, states $\{|\Psi_1^0\rangle\}$ with a single f electron at each site, and second, states $\{|\Psi_2^0\rangle\}$ with admixtures of zero and double f occupation. The energies of the $|\Psi_2^0\rangle$'s are higher than the energies of the $|\Psi_1^0\rangle$'s by amounts proportional to U . In the EKL ($U \rightarrow \infty$) the statistical weights of the $|\Psi_2^0\rangle$'s obviously vanish. Moreover, the creation or annihilation of s electrons, which must be taken into account with regard to s -electron Green's functions of the KLM, do not connect the $|\Psi_1^0\rangle$'s with the $|\Psi_2^0\rangle$'s. Hence, in the EKL only the states $\{|\Psi_1^0\rangle\}$ are relevant. The number of f electrons at each site is effectively fixed to one: $n_{i\uparrow}^f + n_{i\downarrow}^f = 1$.

Based on this, an effective Hamiltonian \bar{H}'' can be formulated, which describes only the relevant states of \bar{H}' in the EKL. Using $n_{i\uparrow}^f + n_{i\downarrow}^f = 1$, several terms of \bar{H}'

can be neglected. Since H_0^U is the only diverging term, there cannot be any finite effective interactions that are omitted this way. H_{ch} can be neglected completely. H_{hop} reduces to the constant $-N \sum_k W_{kk}$, N being the number of lattice sites. The coupling constants simplify to

$$W_{k'k} \xrightarrow{\text{EKL}} \frac{2V_{k'}V_k^*}{U} \quad (22)$$

$$\text{and } J_{k'k} \xrightarrow{\text{EKL}} \frac{8V_{k'}V_k^*}{U}. \quad (23)$$

Taking (22) and (23) into account, H_{dir} exactly vanishes. Neglecting the Hubbard term ($U \sum_i n_{i\uparrow}^f n_{i\downarrow}^f$) as it describes double f occupation, the effective Hamiltonian in the EKL is finally given by

$$\bar{H}'' = \sum_{k\sigma} \epsilon_k n_{k\sigma} + H_{\text{ex}} + N\epsilon_f - N \sum_k W_{kk}. \quad (24)$$

Apart from constants, \bar{H}'' corresponds to the Kondo lattice model H_{KLM} . As there are no f -electron fluctuations, the spin operators \mathbf{S}_i in H_{ex} now describe localized quantum-mechanical spins of magnitude $1/2$.

As $V/U \xrightarrow{\text{EKL}} 0$, for the generator one has $S \xrightarrow{\text{EKL}} 0$. Therefore, the unitary Schrieffer-Wolff transformation reduces to an identical transformation. Thus, in terms of relevant states and disregarding unimportant constants, we have proven

$$H_{\text{PAM}} \xrightarrow{\text{EKL}} H_{\text{KLM}}. \quad (25)$$

The coupling constants of the KLM are given by (23).

Only very recently the long-standing issue of the large Fermi volume for a nonmagnetic Fermi-liquid state of the Kondo lattice model was solved by Oshikawa by means of a nonperturbative topological proof of Luttinger's theorem¹¹. Oshikawa's result represents the first proof of the large Fermi volume for arbitrary dimensions and coupling strengths after a number of special results had been achieved (variational results¹², proof for strong-coupling limit in one dimension¹³, proof for infinite dimensions⁹, general proof for one dimension¹⁴). The exact mapping of the periodic Anderson model to the Kondo lattice model in the extended Kondo limit implies immediately another general proof, which is more direct than the one given by Oshikawa.

To be explicit, for the PAM the Luttinger theorem¹⁰ states that the Fermi volume of a nonmagnetic Fermi-liquid state is equal to the sum of s and f electrons¹⁵:

$$N_s + N_f = 2 \sum_{qk} \theta(\mu - \eta_k^q) \equiv V_F. \quad (26)$$

η_k^q ($q = 1, 2$) are the eigenvalues of the matrix

$$\begin{pmatrix} \epsilon_k & V_k \\ V_k^* & \epsilon_f + \Sigma_k(0) \end{pmatrix}, \quad (27)$$

where $\Sigma_k(\omega)$ is the proper selfenergy of the PAM. Straightforward rearrangements lead to:

$$N_s + N_f = 2 \sum_k \left[\theta(\mu - \epsilon_k) + \theta \left(\alpha - \frac{|V_k|^2}{(\mu - \epsilon_k)} \right) \right] \quad (28)$$

$$\text{with} \quad \alpha = \mu - \epsilon_f - \Sigma_k(0). \quad (29)$$

Eqs. (28) and (29) are analogous to the ones obtained for the special case of infinite dimensions⁹. As in Ref. 9 the three cases of less, equal, and more than half filling have to be distinguished:

$$(\alpha < 0) \quad N_s + N_f = 2 \sum_k \theta(\mu - \epsilon_k - \Sigma_{s,k}(0)) \quad (30)$$

$$(\alpha = 0) \quad N_s + N_f = 2N \quad (31)$$

$$(\alpha > 0) \quad N_s + N_f = 2N + 2 \sum_k \theta(\mu - \epsilon_k - \Sigma_{s,k}(0)) \quad (32)$$

$\Sigma_{s,k}$ is the s -electron selfenergy as defined by an appropriate Dyson equation of the s -electron Green's function,

$$G_{s,k}(\omega) = \frac{1}{\omega - \epsilon_k + \mu - \Sigma_{s,k}(\omega)}. \quad (33)$$

It is related to the proper selfenergy $\Sigma_k(\omega)$ by

$$\Sigma_{s,k}(\omega) = \frac{|V_k|^2}{\omega - \epsilon_f + \mu - \Sigma_k(\omega)}. \quad (34)$$

According to the exact mapping of the PAM to the Kondo lattice model the s -electron selfenergy of the PAM becomes identical to an analogously defined s -electron selfenergy of the KLM in the extended Kondo limit

$$\Sigma_{s,k} \xrightarrow{\text{EKL}} \Sigma_{s,k}^{\text{KLM}}. \quad (35)$$

Hence, Eqs. (30)-(32) with $\Sigma_{s,k}$ replaced by $\Sigma_{s,k}^{\text{KLM}}$ represent the analogue of the Fermi-surface sum rule for a non-magnetic Fermi-liquid state of the Kondo lattice model. The Fermi volume includes the number N_f of localized spins. It is clear that for a magnetic Fermi-liquid state the corresponding Fermi-surface sum rule of the PAM similarly maps to the Kondo lattice model.

In summary, we have proven the exact mapping of the periodic Anderson model in the extended Kondo limit to the Kondo lattice model for any coupling constant J . As a consequence a direct proof of the large Fermi volume of the KLM for a nonmagnetic Fermi-liquid state could be given. Based on the mapping, further analytical and computational results for the KLM can be obtained in future.

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